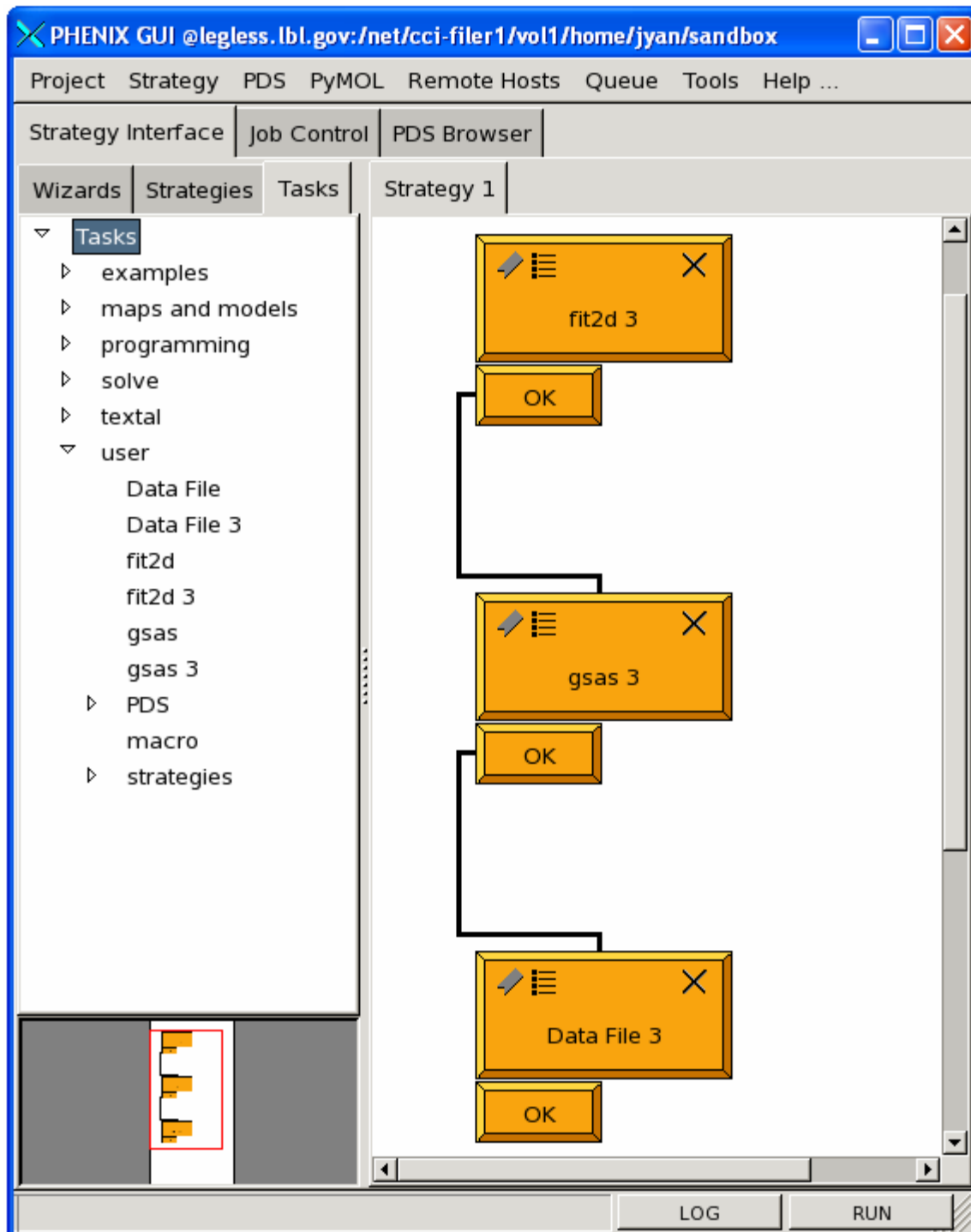


Monthly Report –October, 2006

My work in the last month focused on the multiple raw data input in the fit2d task, input parameters for GSAS, wavelength change for GSAS, etc.



The users can add more raw data files to the file list below along with the corresponding pressure values (temperature values). All of these raw data file are supposed to be collected under the same experimental parameter. The input wavelength is used for GSAS analysis

fit2d_3 Input Parameters

Save Close

INPUT THE .MAR FILES

File name	PRESSURE VALUE	
File 1 me/jyan/sandbox/LaB6sept12_001.gsas	130.0	Parameter Group Options
File 2 yjan/sandbox/LaB6sept12_001.mar3450	120.0	Parameter Group Options
File 3 me/jyan/sandbox/LaB6sept12_001.gsas	110.0	Parameter Group Options

BEAM CENTER

X_COORD (Pixel)	Y_COORD (Pixel)	WAVELENGTH(ANSTRONG)
Value 1819.101	1823.927	0.6199

DISTANCE, ROTATION, AND TILT

DISTANCE (mm)	ROTATION (Degree)	TILT (Degree)
Value 380.1731	-35.89497	-0.317431

The right instrumental file can be input below for GSAS along with the background function parameters, element information, profile editing, etc.

gsas_3 Input Parameters

Save Close

Instrument File

BACKGROUND PARAMETERS

BKGD PARA 1	BKGD PARA 2	BKGD PARA 3	BKGD PARA 4	BKGD PARA 5
Value 0.0	0.0	0.0	0.0	0.0

BACKGROUND PARAMETERS

BKGD PARA 6	BKGD PARA 7	BKGD PARA 8	BKGD PARA 9	BKGD PARA 10
Value 0.0	0.0	0.0	0.0	0.0

TYPE, X, Y, Z, FRAC

SPACE GROUP	ELEMENT_1	FLAG_1	ELEMENT_2	FLAG_2
Value p m -3 m	la 0 0 1	i 0.00858	B 0.5 0.5 0.2021 1	i 0.009

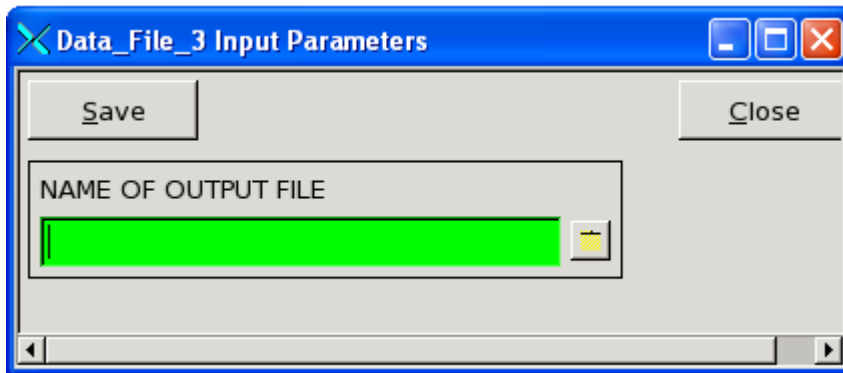
PROFILE EDITING OPTIONS_1

GU GV GW	IX LY trns	asym shft GP
Value 0 0 20	0 10 0	0 0 0

PROFILE EDITING OPTIONS_2

GU	GV	GW	LX	LY	trns
Value n	n	n	n	n	n

The unit cell information for all the input raw data files will be saved in the output file here.



Before the multi raw data file input, the unit cell volumes of one LaB6 .mar file were calculated in three different ways, CEAD, Linux command-line mode, and Windows GUI. The results below show that the result from CEAD is correct.

CEAD	71.914
Linux Command-line	71.914
Window GUI	71.915

2. Next step.

- (1) There are still some works for the multiple raw data file input to be done
- (2) The over-flow problem in the fit2d output data file is under my consideration.